Ioana Cozmuta

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SUMMARY OF QUALIFICATIONS

- Extensive experience in Computational Chemistry and Applied Physics applied to Material Science, Bio- and Nanotechnology, Biophysics, Aerospace Engineering.
- Independent, organized, resourceful, inventive, reliable, responsible.
- Good leadership and oral/written communication skills, highly energetic.
- Extensive experience in conducting independent research, presenting results and writing proposals. Committed to interdisciplinarity.
- Extensive experience with large-scale parallel computing, data analysis of Tera-bytes of data, visualization.
- Strong problem solving ability, very good analytical and numerical skills, statistics and error analysis.
- Proficient in C, Fortran, Matlab, Mathematica, Perl, TCL/TK, C-shell; Unix, Linux and Windows operating systems.
- Very good knowledge of computational chemistry software packages: Amber, NAMD, VMD, Grasp-Reax Force Field, Lammps, Gaussian, Cerius2, InsightII and CMDF.
- Extensive experience with finite differences methods applied to multi-phase time dependent transport equations in porous media.
- Very good experimental skills and broad based knowledge of experimental techniques in applied physics and material science.
- Native speaker of Romanian, proficient in English, Dutch, German and French

ACADEMIC DEGREES

Ph.D., Physics (2001)

University of Groningen **Groningen, The Netherlands** **1997-2001**

- Thesis title: “Radon generation and transport, a journey through matter”
- Achieved 37 credit points (required: 24)
- Advisor: prof. R.J. de Meijer and dr. E. R. van der Graaf,

M.Sc., Biophysics/Physics (1996)

Babes Bolyai University **Cluj-Napoca, Romania** **1995–1996**

- Thesis title: “Radon Retrospective Measurements”
- GPA: 10.0/10.0 (4.0/4.0)
- Advisor: prof. C. Cosma

B.Sc., Physics (1995)

Babes Bolyai University **Cluj-Napoca, Romania** **1991-1995**

- Thesis title: “Nuclear Radiation in Medical Physics”, GPA: 9.16/10.0 (3.7/4.0)
- Advisor: prof. C. Cosma
- Graduated the University Pedagogical Seminar, GPA: 9.25/10.0 (3.7/4.0)

Employment History

05/2006-present

Senior Research Scientist, Space Technology Division, Reactive Flow Environment Branch; NASA Ames Research Center, Moffett Field, CA

Projects: Atomistic scale simulations using reactive and non-reactive potentials relevant to hypersonic reentry employing Molecular Dynamics and Grand Canonical Monte Carlo simulations of gas adsorption on SiO_2 under hypersonic conditions and reactive force field simulations for surface *catalicity* of SiO_2

03/2003-05/2006

Scientist, Center for Nanotechnology and Genome Research Facility; NASA Ames Research Center, Moffett Field, CA

Projects: Atomistic scale simulations for the rational design of a DNA sequencer

Hybrid MD-PNP simulations of ionic currents through biological and solid-state nanopores

Quantum and atomistic study of voltage dependence reactivity of DNA phosphate groups for building DNA strands

Reactive potential based atomistic simulations to study pH dependence of solid-state nanopore surface chemistry

Development of a TCL/TK based graphical interface for nanopore simulations.

05/2002-03/2003

Research Scientist, School of Medicine, Department of Chemistry; Stanford University, Palo Alto, CA

Projects: Atomistic simulations of the alpha hemolysin protein channel relevant to DNA translocation.

Code development for bio-informatics projects to analyze hybridization data from high-density oligonucleotide arrays.

04/2001-05/2002

Research Scientist, Material and Process Simulation Center; California Institute of Technology, Pasadena, CA

Projects: Multiscale, hierarchical modeling of barrier properties of polymeric membranes: adsorption and diffusion of small molecules on polymeric membranes and surfaces

Atomistic scale simulations to model polymer-clay nanocomposites

Atomistic scale simulations to investigate the process of nucleation in alkane mixtures and mechanisms of inhibition

Statistical ensembles and error analysis

02/2000-03/2001

Visiting Scientist, Material and Process Simulation Center; California Institute of Technology, Pasadena, CA

Projects: Atomistic and Monte Carlo simulations of sorption properties of barrier polymeric membranes

01/1997-03/2001

Research Assistant, Institute of Nuclear Physics, University of Groningen; Groningen, The Netherlands

Projects: Analytical and numerical implementation of radon-related transport equations.

Statistical and error analysis of simulation and experimental data

Coupling of radon transport model with a model for the simulation of concrete microstructure.

Measurements of radon release rates from porous media

Determine the influence of various physical and structural properties of building materials on radon release rates via experiments and computer simulations

Design, optimization (sensitivity analysis), calibration and testing of a method to determine the radon diffusion coefficients and porosities in building materials (porous media)

Investigation of various methods for inhibiting radon release from building materials: surface covering and design of low-radon emanating building materials.

01/1996- 12/1996

Physicist, Environmental Protection Agency; Baia Mare, Romania

Projects: Development of pollution models including radioactive and non-radioactive sources

Setup and calibration of a mobile lab for in situ measurement of atmospheric pollution and meteorological parameters

Research Experience

- Atomistic scale simulations of wide variety of systems: protein channels, DNA and RNA molecules, ionic solutions, poly-electrolites, solid state nanopores, polymeric membranes, hydrocarbon mixtures, clay-polymer nanocomposites, DNA/RNA in solid state nanopores, gas-surface interactions, teflon, nanowires.
- Development and application of new computational modeling capabilities to calculate ionic currents and ionic current blockades due to nucleic acid translocation through biological and solid-state nanopores.
- Accelerated (Steered) Molecular Dynamics techniques to reconstruct the Potential of Mean Force (PMF) for DNA translocating through nanopores.
- Pioneering work to establish a computational method for surface functionalization of a nanopore DNA sequencer. Developed a suite of scripts and algorithms for implementation under a common TCL/TK graphical interface.
- Multiscale modeling development and application: hybrid MD-PNP model to calculate ionic currents in protein channels.
- Development of quantum (DFT, HF, MP2) based empirical parameters for classical and reactive force fields.

- Multiscale modeling development and application: MD-MC applied to the study of barrier properties of polymeric membranes.
- Generation of polymeric samples and statistical analysis
- Method development and testing to calculate solubility and diffusion coefficients of gas solutes in polymeric membranes.
- Atomistic scale simulations to investigate the process of nucleation in alkane mixtures and mechanisms of inhibition.
- Performed extensive studies of hybrid (organic-inorganic) systems. Simulations of clay exfoliation as function of surfactant properties, clay-polymer and clay-electrolyte interactions.
- Developed analytical and numerical models for transport phenomena in porous solids and coupled the microstructure time evolution model with the transport model. Error analysis.
- Performed extensive experimental measurements on radon release rates from concrete and validated the data with the coupled microstructure-transport numerical scheme. Error and statistical analysis.
- Assessed implications of the developed model on indoor-air radon concentrations as correction for the Radiation Performance Index Standard used in the Dutch building codes by the government.

Scholarships and awards

- NASA funded postdoctoral fellowship, Stanford University (2002-2003)
- Ubbo Emmius Graduate Research Fellow, University of Groningen, The Netherlands (1997-2001)
- FANTOM award, Visiting Scholar at MSC-CALTECH, Pasadena, CA (2000)
- FANTOM scholarship, Visitor, Department of Civil Engineering, University of Texas at Austin, Austin, TX (1998)
- FANTOM scholarship to attend the International “Accelerator Physics” School at CERN, Geneva, Switzerland, 1998
- FANTOM scholarship to attend the FANTOM schools in Tecklenburg (Germany), Gent (Belgium), Ameland (The Netherlands), Egmond aan Zee (The Netherlands)
- Ministry of Education undergraduate scholarship, Romania (1991-1996).

Professional Activities

- Experience with grant/proposal writing (Co-PI and PI status)
- Initiated collaboration (ongoing) between Caltech, MIT and Sandia National Lab for further development and application of Grasp-ReaxFF simulations.
- Largest single user on the Columbia Supercomputer, NASA Ames Research Center.
- Invited Demo for the NASA booth at the Supercomputing conferences, SC04, SC05 and SC06.
- NASA SBIR grant reviewer (2002-2005)

- Participated in DARPA PI meetings (2002-2003)
- Supervising activity of one MSc and one PhD student and two summer interns.
- Initiated collaboration with the Department of Civil Engineering, University of Tokyo and Department of Civil Engineering, University of Texas at Austin for simulations related to concrete microstructure (1998-2000).
- Co-organizer of the Medical Physics European Conference, Cluj-Napoca, Romania, November 1995. Obtained funding from industry; edited the proceedings, other administrative assignments.

Publications

I. Cozmuta and H. Mehrez, *DNA modeling: from ab initio to empirical*, invited article to the Journal of Computational and Theoretical Nanoscience, in press.

I.Cozmuta and V. Stolc, *Fast scanning method using SMD simulations for surface functionalization of nanopore sequencers: 1. Method description 2. Application to natural amino acids*, in preparation.

I. Cozmuta, M. Blanco and W. A. Goddard, *Atomistic predictions relevant to exfoliation of layered clays to form nanocomposites"*, in preparation.

I. Cozmuta, M. Blanco and W. A. Goddard, *Gas sorption and Barrier Properties of Polymer Membranes from MD and MC simulations*, Journal of Physical Chemistry B, in press.

I.Cozmuta and V. Stolc, *Steered Molecular Dynamics Simulations for Rational Design of a Nanopore DNA Sequencer*, Journal of Computational and Theoretical Nanoscience, in press

I. Cozmuta, "*Molecular mechanisms of gas surface interactions in hypersonic flow"*, in preparation.

I. Cozmuta and V. Stolc, *Fast MD scanning method for surface derivatization of a protein ring sequencer*, Proceedings of the Biophysical Society Meeting, Salt Lake City, UT, 2006.

I. Cozmuta, J. T. O'Keeffe, D. Bose and Viktor Stolc, *Hybrid MD-Nernst Planck model of α-hemolysin conductance properties,* Molecular Simulations, vol. 31, no. 2-3, 2005.

I. Cozmuta, J. T. O'Keeffe and Viktor Stolc, *Molecular dynamics approach to calculate α-hemolysin ion currents,* Proceedings of the Biophysical Society Meeting, Baltimore, MD, 2004.

I. Cozmuta, J. T. O'Keeffe, D. Bose and Viktor Stolc, *Hybrid MD-PNP simulations of the α-hemolysin open channel ionic current,* Proceedings of the Nanotechnology 2004 conference, Boston, MA, 2004.

I. Cozmuta, E.R. van der Graaf and R. J. de Meijer, *Moisture Dependence of Radon Transport in Concrete: Measurements and Modeling*, Health Physics, vol. 85, no. 104, October 2003.

I. Cozmuta, M. Brock, J. T. O'Keeffe and Viktor Stolc, *Nanopore sensors for detection and analysis of biological polymers,* Proceedings of the DARPA PI meeting, Monterey, CA, September 2003.

I. Cozmuta, J. T. O'Keeffe and Viktor Stolc, *Towards an MD simulation of ion currents in the alpha hemolysin channel,* Proceedings of the IEEE, San Francisco, CA, August 2003.

I. Cozmuta, J. T. O'Keeffe and Viktor Stolc, *Ionic signature of the alpha hemolysin channel,* Proceedings of the DARPA PI meeting, Santa Barbara, CA, February, 2003.

I. Cozmuta and Viktor Stolc, *Ionic signature of Nanopores,* Proceedings of the DARPA PI meeting, Portland, OR, August 2002.

I. Cozmuta, A. Strachan, M. Blanco and W. A. Goddard III, *Exfoliation of Montmorillonite for Clay Nanocomposites*, Proceedings of the MSC 2002 Conference, Caltech, Pasadena, CA, 29-30 March 2002.

I. Cozmuta, E.R. van der Graaf, *Modeling radon transport in concrete*, Proceedings of the MSC 2001 Conference, Caltech, Pasadena, CA, 29-30 March 2001.

I. Cozmuta, E.R. van der Graaf, *Methods for measuring diffusion coefficients of radon in building materials*, Science of the Total Environment, vol. 272, no. 1-3, pp: 323-335, May 2001.

I. Cozmuta, E.R. van der Graaf, R.J. de Meijer, *Moisture dependence of radon release from concrete,* KVI Annual Report 2001, Groningen, The Netherlands.
I. Cozmuta, E.R. van der Graaf, *Aspects of radon transport in concrete*, Proceedings of the MSC 2000 Conference, Caltech, Pasadena, CA, 23-24 March 2000.
I. Cozmuta, E.R. van der Graaf, R.J. de Meijer, *Radon redu ction by surface covering: a new approach*, KVI Annual Report 2000, Groningen, The Netherlands.
I. Cozmuta, E.R. van der Graaf, R.J. de Meijer, *Modeling concrete's structural parameters*, KVI Annual Report 2000, Groningen, The Netherlands.
I. Cozmuta, E.R. van der Graaf, R.J. de Meijer, *Experimental study on the moisture dependence of radon-release rates of concrete*, KVI Annual Report 1999, Groningen, The Netherlands.
I. Cozmuta, E.R. van der Graaf, R.J. de Meijer, *Concrete composition and radon release*, KVI Annual Report 1999, Groningen, The Netherlands.
I. Cozmuta, E.R. van der Graaf, *Effects of surface covering on radon exhalation rates from concrete*, Proceedings of the AARST International Radon Symposium, 14-16 September 1998, Cherry-Hill, NJ.
I. Cozmuta, E.R. van der Graaf, R.J. de Meijer, *Measurements of the radon-diffusion coefficient in concrete using a cylindrical geometry*, KVI Annual Report 1998, Groningen, The Netherlands.
I. Cozmuta, E.R. van der Graaf, R.J. de Meijer, *Radon exhalation of building materials: effect of surface covering*, KVI Annual Report 1997, Groningen, The Netherlands.
I. Cozmuta and J. Ferenczi, *Radioactivity, a geological chronometer*, Proceedings of the National Physics Conference, Baia Mare, Romania, 1996.
I. Cozmuta and J. Ferenczi, *The second cosmic velocity and some parameters of neutronical stars*, Proceedings of the National Physics Conference, Baia Mare, Romania, 1995.

Technical Reports

I. Cozmuta and V. Stolc, *Ionic signature of nanopores: initial assessment for protein channels*, Stanford Internal Report, March 2003.
I. Cozmuta, M. Blanco and W. A. Goddard, *Wax formation and inhibition*, Chevron Corporation Quarterly Report, April 2002.
I. Cozmuta, M. Blanco and W. A. Goddard, *Multi-scale, Hierarchical Modeling of Membrane Barrier Properties: Clay-Surfactant Exfoliation Properties and PDDA/Clay Nanocomposite Structure and Dynamics*, Avery Dennison Quarterly Report, January 2002.
I. Cozmuta, M. Blanco and W. A. Goddard, *Insight into the process of nucleation of small alkanes*, Chevron Corporation Quarterly Report, October 2001.
A. Strachan, **I. Cozmuta**, M. Blanco and W. A. Goddard, *Multi-scale, hierarchical modeling of membrane barrier properties: Kinetic Monte Carlo studies of Gas Diffusion in Polymers and A New Force Field for the Modeling of Clay Nanocomposites*, Avery Dennison Quarterly Report, August 2001.
A. Strachan, **I. Cozmuta**, R. Niemer, M. Blanco and W. A. Goddard, *Multi-scale, Hierarchical Modeling of Membrane Barrier Properties: MD/Monte Carlo Method for the Estimation of Henry's Solubility Constants and Gas Diffusivities in Polymers*, Avery Dennison Quarterly Report, September 2000.
A. Strachan, **I. Cozmuta**, R. Niemer, Y. Zhou, M. Blanco and W. A. Goddard, *Multi-scale, Hierarchical Modeling of Membrane Barrier Properties*, Avery Dennison Quarterly Report, July 2000.
I. Cozmuta, E. R. van der Graaf and R. J. de Meijer, *Moisture dependence of*

radon transport in concrete: measurements and modeling, KVI Internal Report, R124, pp. 1-35, December 2002.

I. Cozmuta and E. R. van der Graaf, *Modeling radon transport in concrete, KVI Internal Report*, R120, pp. 1-56, April 2001.

I. Cozmuta, M van der Pal and E. R. van der Graaf, *Calibration of the NGD-KVI porosimeter and results of initial experiments on aerated concrete samples from TUE*, KVI Internal Report, S75, pp. 1-20, February 2001.

E. R. van der Graaf and **I. Cozmuta**, *NEN5699: Radon Exhalation Rate Intercomparison Results of NGD-KVI,* KVI Internal Report, R119, pp. 1-6, December 1999.

E. R. van der Graaf and **I. Cozmuta**, *Determination of the radon permeability of three membranes received from HYPLAST NV*, KVI Internal Report, S56, pp. 1-15, June 1999.

E. R. van der Graaf, **I. Cozmuta** and R. J. de Meijer, *The influence of 1) dimensions and 2) effectiveness of four-sided coverage of concrete test cubes on the determination of their exhalation rates*, KVI Internal Report, R110, pp. 1-116, May 1999.

I. Cozmuta and E. R. van der Graaf, *Methods for measuring diffusion coefficients of radon in building materials*, KVI Internal Report, R105, pp. 1-28, April 1999.

E. R. van der Graaf and **I. Cozmuta**, *Determination of radon release rate and activity concentrations of natural radionuclides in cellular concrete from the radon cylinder at TUE*, KVI Internal Report, S54, pp. 1-7, April 1999.

E. R. van der Graaf and **I. Cozmuta**, *ERRICCA: Radon Exhalation Rate Intercomparison Results of NGD-KVI,* KVI Internal Report, R111, pp. 1-5, March 1999.

E. R. van der Graaf, **I. Cozmuta**, W. H. van der Spoel and R. J. de Meijer, *Calibration of the KVI instrument to measure radon exhalation rates from building materials under controlled conditions*, KVI Internal Report, R99, pp. 1-46, March 1998.

Additional Publications

J. T. O'Keeffe, **I. Cozmuta,** D. Bose and Viktor Stolc, "*A Predictive MD-Nernst Planck Model of Transport Through Protein Channels: Relating Structure to Ion Current*", Proceedings of the Biophysical Society Meeting, Salt Lake City, UT, 2006.

J. T. O'Keeffe, **I. Cozmuta** and Viktor Stolc, *Polymer translocation through a nanopore: a geometry dependence study,* Proceedings of the IEEE, San Francisco, CA, August 2003.

E.R. van der Graaf, **I. Cozmuta**, R.J. de Meijer, *Moisture dependence of the radon diffusion coefficient of concrete*, KVI Annual Report 2000, Groningen, The Netherlands.

E.R. van der Graaf, **I. Cozmuta** et all, *Moisture dependence of radon exhalation from concrete*, Proceedings of the Third Euro Symposium on Protection against Radon, Liege, Belgium, 21-25 April, 2001.

A. Strachan, **I. Cozmuta**, M. Blanco, W. A. Goddard, R. Bharadwaj and D. Saunders, *Successes and Challenges in First-Principles Modeling of Solubility and Diffusion of Small Molecules through Amorphous Polymers*, Proceedings of the MSC 2001 Conference, Caltech, Pasadena, CA, 29-30 March 2001.

E.R. van der Graaf, **I.Cozmuta**, R.J. de Meijer, *Dutch intercomparison of radon-exhalation measurements*, KVI Annual Report 2000, Groningen, The Netherlands.

E.R. van der Graaf, **I.Cozmuta**, R.J. de Meijer, *Design and calibration of a porosimeter for large samples*, KVI Annual Report 2000, Groningen, The

Netherlands.
E.R. van der Graaf, **I. Cozmuta** et all, *Aspects of Radon in Dutch Building Practice*, Proceedings of the International Building Physics Conference, Eindhoven, The Netherlands, 18-21 September, 2000.
E.R. van der Graaf, **I.Cozmuta**, R.J. de Meijer, *ERRICCA radon-model intercomparison*, KVI Annual Report 1999, Groningen, The Netherlands.
E.R. van der Graaf, **I.Cozmuta**, R.J. de Meijer, *ERRICCA radon-release rate intercomparison*, KVI Annual Report 1999, Groningen, The Netherlands.
C.Edsfelt, **I.Cozmuta**, E.R. van der Graaf, *Radium distribution in soils, analyzed with sequential extraction, and its effect on radon emanation*, KVI Annual Report 1998, Groningen, The Netherlands.
C. Cosma, **I. Cozmuta** and C. Micu, *Some bioindicators of radioactive contamination*, Proceedings of 3rd Symposium of the Croatian Radiation Protection Association with international participation, Zagreb, Croatia, November 20-22,1996.
G. Meesen, **I. Cozmuta**, A. Poffijn, C. Cosma and J. Ferenczi, *Feasibility study of retrospective radon measurements by means of implanted Po-210 in glass,* Proceedings of 3rd Symposium of the Croatian Radiation Protection Association with international participation, Zagreb, Croatia, November 20-22,1996.
C.Cosma, A.Zeriu, **I.Cozmuta**, C.Micu*, Bioindicators of environmental radioactive contamination*, Proceedings of IXth Conference of Medical Physics, Trieste, Italy, 1996.
C.Cosma, A.Zeriu, **I.Cozmuta**, C.Micu, *Some natural indicators of radioactive pollution*, Proceedings of IRPA Conference, Warsaw, Poland, September ,1996.
C. Cosma, A. Zeriu, **I. Cozmuta**, C. Micu, *Bioindicators of Radioactive Environmental Contamination*, Proceedings of the Symposium "10 Years on Chernobyl", Targu Mures, Romania,1996.
C. Cosma, A. Duca, **I. Cozmuta**, D. Ristoiu, *Application of Radon Measurements on Earthquake Prediction*, Proceedings of the National Physics Conference, Oradea, Romania, 1996.
C. Cosma, A. Zeriu, C. Himeinschi, I. Pop, **I. Cozmuta**, *Some aspects of Cs-137 Depositions in Romania after the Chernobyl Accident*, Proceedings of the National Physics Conference, Baia Mare, Romania, December, 1995.
C. Cosma, I. Pop, **I. Cozmuta**, C. Micu, *Measurements on Cs-137 in Romania*, Proceedings of the Medical Physics Conference, Cluj-Napoca, Romania, November, 1995
C.Cosma, I.Pop, **I.Cozmuta**, C.Micu, S.Ramboiu, *Some aspects of Cesium deposition in Transilvania/Romania*, Proceedings of the IRPA Conference, Portoros, Slovenia, September, 1995.

Conference presentations

- SC2006 High Performance Computing, Networking and Storage Conference, **presentation and poster for the NASA booth**, Tampa, FL, November, 2006.
- Biophysical Society 50th meeting, **oral and poster presentation**, Salt Lake City, UT, February 2006.
- "*Fist principles modeling of nanomaterials*", **invited presentation**, NanoStellar Inc., Menlo Park, CA, January 2006.
- SC2005 High Performance Computing, Networking and Storage Conference, **presentation and poster for the NASA booth**, Seattle, WA, November, 2005.
- SC2004 High Performance Computing, Networking and Storage Conference, **presentation and poster for the NASA booth**, Pittsburgh, PA, November 6-12, 2004.

- The Nanotechnology Conference, Nanotech 2004, **oral presentation**, Boston, MA, March 20004.
- Biophysical Society 48th meeting, **oral presentation**, Baltimore, MD, February 2004.
- DARPA PI meeting, **oral and poster presentation**, Monterey, CA, September 2003.
- IEEE Conference, **oral presentation**, San Francisco, CA, August 2003.
- DARPA PI meeting, **poster presentation**, Santa Barbara, CA, February 2003.
- DARPA PI meeting, **poster presentation**, Portland, OR, August 2002.
- Avery Dennison Corporation, **oral presentation** -project summary, Pasadena, CA, April 2002.
- California Institute of Technology**, oral presentation**, MSC 2001 Annual Conference, 29-30 March 2001.
- California Institute of Technology**, oral presentation**, MSC 2001 Annual Conference, 23-24 March 2000
- Technical University of Athens, Greece, **invited keynote presentation**, ERRICA Workshop "Radon in the living environment", 19-23 April 1999.
- AARST International Radon Symposium**, oral and poster presentation**, NJ, 14-16 September 1998
- North University of Baia Mare, Romania, **oral presentation**, EVRIKA National Physics Conference, December 1996.
- International Radiation Protection Agency Conference**, oral presentation**, Warsaw, Poland, September 1996.
- International Radiation Protection Agency Conference, **oral presentation,** Portoros, Slovenia, September 1995.